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Feasibility Study on the Use of Visible and Near-Infrared Spectroscopy Together with Chemometrics To Discriminate between Commercial White Wines of Different Varietal Origins

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The use of visible (vis) and near-infrared spectroscopy (NIR) was explored as a tool to discriminate between samples of Australian commercial white wines of different varietal origins (Chardonnay and Riesling). Discriminant models were developed using principal component analysis (PCA), principal component regression (PCR), and discriminant partial least-squares (DPLS) regression. The samples were randomly split into two sets, one used as a calibration set ($n = 136$) and the remaining samples as a validation set ($n = 133$). When used to predict the variety of the validation set samples, the DPLS models correctly classified 100% of Riesling and up to 96% of Chardonnay wines. These results showed that vis–NIR might be a suitable and alternative technology that can be easily implemented by the wine industry to discriminate Riesling and Chardonnay commercial wine varieties. However, the relatively limited number of samples and varieties involved in the present work suggests caution in extending the potential of such a technique to other wine varieties.

KEYWORDS: Visible; near-infrared spectroscopy; white wine; classification; discrimination; PCA; PCR; DPLS

INTRODUCTION

Determination of food authenticity is one of the most important issues in food quality control and safety. The authenticity of wine is regulated by strict guidelines laid down by the responsible national authorities, which may include official sensory evaluation, chemical analysis, and examination of the records kept by the wine producer (*1*). Wine identification, or classification, mainly in terms of variety and geographical region of origin, has received increasing attention during the past 10 years using multivariate statistical techniques (*1–3*). Recently, the use of multivariate statistical techniques on chemical and sensory data has gained increasing attention as a means to classify wines from different geographical regions and to describe similar and discriminating sensory and chemical characteristics (*1*).

Group classification of wine authenticity has been attempted using several different types of compositional data including volatile compounds (*4*), aroma components (*5*), and minerals and trace elements (*6*), as well as phenolic compounds and amino acids (*1*). All of these methods require sophisticated and expensive analytical equipment such as high-performance liquid chromatography (HPLC), mass spectrometry (MS), gas–liquid chromatography (GLC), and atomic absorption spectroscopy (AAS).

Near-infrared spectroscopy (NIR) was originally developed to provide a rapid measurement of the composition of grains and oilseeds (*7*). NIR has emerged in the past 30 years as a method to predict the quality of different foods and agricultural products due to the speed of analysis, minimum sample preparation, and low cost (*7–9*). Most of the established methods have involved the development of NIR calibrations for the quantitative prediction of composition in food (*8*).

This was a rational strategy to pursue during the initial stages of its application, given the type of equipment available, the state of development of the emerging discipline of chemometrics, and the overwhelming commercial interest in solving such problems (*10–12*). One advantage of NIR is that it can record the response of the molecular bonds of its chemical constituents to the near-infrared spectrum (e.g., O–H, N–H, and C–H bonds) and thereby build a characteristic spectrum that behaves as a "fingerprint" of the sample (*10, 13*). This opens the possibility of using spectra to determine complex attributes of foods including organoleptic scores or even sensory characteristic (*10*). In addition, the application of multivariate statistical techniques such as principal component analysis (PCA) or discriminant analysis provides the possibility to use and

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7704 *J. Agric. Food Chem.,* Vol. 51, No. 26, 2003

Cozzolino et al.

understand the spectral properties of the sample and make a classification without the need for chemical data.

NIR has been examined to assess its suitability as a tool for the authentication of fat substitutes in milk (*14*), authentication and detection of contamination in various foods (*11*), discrimination between fresh and frozen beef (*15, 16*), discrimination between beef and kangaroo meat (*17*), authentication of asparagus varieties (*18*), contamination of fish meal with bone and meat meal (*19*), discrimination among different feeding regimens of cattle (*20*), and in olive oil adulteration (*21*).

The spectral properties of both grapes and wines have been used as a means of determining the gross chemical composition (e.g., alcohol, total acidity, pH, and color) by the wine industry in Australia (*22, 23*). These same spectral properties might provide a means of characterizing complex features of wine quality including aroma, stability, oxidation, and grading, as well as possibly assisting in determining the relationship between the chemical composition and sensory characteristics of wine. There are several reports in the literature on the use of multivariate statistical techniques combined with sensory characteristics and chemical composition data for the classification of commercial wines according to their geographical origin (*24–26*). However, no reports were found in the literature in relation to the use of NIR for wine varietal identification, authentication, or discrimination. The Australian wine industry regulations (*36*) state that a single varietal wine must contain a minimum of 85% of the variety as claimed on the label. It is therefore possible that some of the samples were not 100% of the variety as claimed.

The aim of this work was to investigate the potential of NIR as a rapid and low-cost technique to discriminate between two commercial white wine varieties (Riesling and Chardonnay) using their spectral properties without depending on chemical composition and sensory characteristics.

MATERIALS AND METHODS

Samples. Commercially available bottles of Australian wine indicated by their labels to be Riesling ($n = 144$) and unwooded Chardonnay ($n = 125$) were sourced from a broader wine flavor study (H. Smyth, Ph.D. thesis, in preparation). The wines showed a diversity of sensory characteristics and ranged in vintage from 1993 to 2002 for the Riesling and from 1998 to 2002 for the Chardonnay. The Riesling wines ranged in price from less than \$8 A to more than \$35 A per bottle and were from several viticultural regions within the states of South Australia (60%), Victoria (15%), Western Australia (10%), New South Wales (5%), and Tasmania (5%), with the remainder being nonregional blends (5%). The commercial unwooded Chardonnay wines ranged in price from less than \$10 A to more than \$20 A per bottle and were from a variety of regions within South Australia (61%), Victoria (22%), Western Australia (11%), and New South Wales (6%). These samples comprised a set of wines with varying characteristics due to different regions and ages. Although replicate bottles from an individual commercial label were used for scanning, only one bottle from each label and variety (Riesling, $n = 20$; Chardonnay, $n = 17$) were analyzed for alcohol content, specific gravity, pH, free and total sulfur dioxide, titratable acidity, glucose plus fructose, total dry extract, and volatile acidity using standard laboratory methods at the AWRI Analytical Service (*27*). **Table 1** shows the mean and standard deviation of the chemical composition of both sets of varietal wines. Chemical compositional data were analyzed for differences in the mean values for the two groups of varieties using a Student *t* test ($p < 0.05$) using JMP software (version 5.01, SAS Institute Inc., Cary, NC).

Spectroscopic Measurements. Samples taken from freshly opened bottles of wine were scanned in transmission mode (400–2500 nm) using a scanning monochromator FOSS NIRSystems6500 (FOSS NIRSystems, Silver Spring, MD). Spectral data were collected using Vision software (version 1.0, FOSS NIRSystems). Samples were

Table 1. Mean, Standard Deviation, and Significance of Differences in Chemical Composition for Riesling and Chardonnay Wine Samples[a]

	Chardonnay	Riesling	significance of difference
alcohol (%)	13.2 (0.5)	12.2 (0.6)	*
specific gravity	1 (0.001)	0.99 (0.001)	*
pH	3.3 (0.1)	3.1 (0.1)	*
SO_2, free (mg L^{-1})	24.5 (6.5)	18.5 (6.3)	NS
SO_2, total (mg L^{-1})	125.3 (22.4)	107.5 (23.2)	NS
TA, to pH 8.2 (g L^{-1})	6.6 (0.6)	6.6 (0.5)	NS
glucose + fructose (g L^{-1})	3.9 (1.6)	4.0 (2.1)	NS
dry extract (g L^{-1})	25.3 (2.4)	22.6 (1.9)	*
VA as acid (g L^{-1})	0.40 (012)	0.33 (0.1)	NS
N	17	20	

[a] TA, titratable acidity; VA, volatile acidity; *N*, number of samples analyzed by wet chemistry; figures in parentheses, standard deviations; NS, not significant; *, $p < 0.05$.

scanned in a rectangular cuvette in a 1 mm path length (part no. 7063-1, FOSS NIRSystems) and pre-equilibrated at 33 °C during 3 min before scanning. Spectral data were stored as logarithm of the reciprocal of transmittance [$\log(1/T)$] at 2 nm intervals. The spectrum of each sample was the average of 32 successive scans (1050 data points). Because the samples were sourced from a complex sensory experimental program, the scanning of samples took place over several months, first with the Riesling (November 2002–January 2003), followed by the Chardonnay samples (January–May 2003).

Data Analysis and Interpretation. Spectra were exported from the Vision software in NSAS format to The Unscrambler software (version 7.5, CAMO ASA, Oslo, Norway) for chemometric analysis. All of the spectra ($n = 269$) were examined for unusual samples using PCA on both the raw spectra and the second derivative after processing. The second derivative was used to reduce baseline variation and enhance the spectral features, and it was performed using Savitzky–Golay derivation and smoothing (20 point and second-order filtering operation) (*28*). After outlier removal, the sample set was divided at random into two sets, namely, calibration and validation sets, with each comprising 72 Riesling and 64 (or 61, respectively) Chardonnay wine samples. PCA was performed before principal component regression (PCR) and discriminant partial least-squares (DPLS) classification models were developed. PCA is a method of data reduction that constructs new uncorrelated variables, known as principal components (PCs), that are linear combinations of the original ones. The PCs account as much as possible for the variability in the original variables (*29, 30*). PCA was used to derive the first 20 principal components from the spectral data to ensure that all of the variability is considered by the analysis and was used to examine the possible grouping of samples and the presence of outliers (*29, 30*).

Discriminant models were developed using the DPLS regression technique as described elsewhere (*8, 20, 29, 31*). In this technique, each sample in the calibration set is assigned a dummy variable as a reference value, which is an arbitrary number if the sample belongs to a particular group or if it does not—in this case samples of Riesling wines were assigned a numeric value of 1 and Chardonnay, 2.

The DPLS model is then developed by regression of the spectral data against the assigned reference value (dummy variable). The methods of regression used were PCR and DPLS, both with cross-validation and developed using either the raw spectra or after second derivative (*29*). Cross-validation estimates the prediction error by splitting the calibration samples into groups (four in this case). One group was reserved for validation, and the remaining groups were used for calibration. The process was repeated until all groups had been used for validation once. The optimum number of calibration factors for each model was selected on the basis of predicted residual sum of squares (PRESS). In both PCR and DPLS calibration models, statistics calculated included the standard error of calibration (SEC), the coefficient of determination in calibration (R^2_{cal}), and the standard error in cross-validation (SECV). To perform the calibration, PCR and DPLS regression models were developed using five spectral regions: visible,
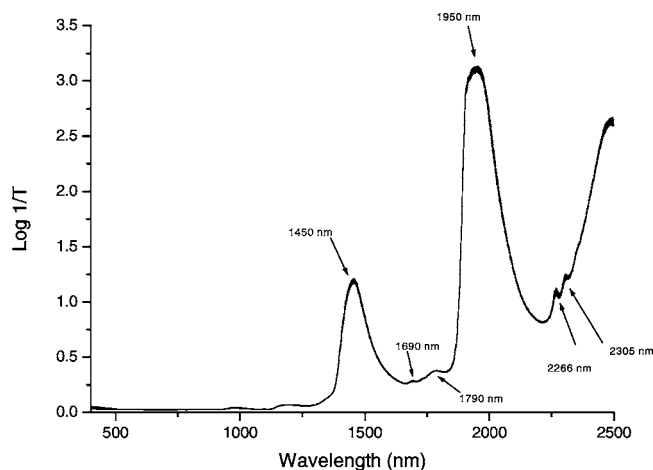
Vis-NIR Varietal Wine Discrimination

J. Agric. Food Chem., Vol. 51, No. 26, 2003 **7705**

Figure 1. Visible and near-infrared spectra of white wine samples analyzed.

Figure 2. Standard deviation of the second derivative of the mean spectrum of the white wine samples.

400−700 nm (visible region); 400−1100 nm (visible + NIR), near-infrared 1100−2500 nm; visible and near-infrared region, 400−2500 nm (whole spectrum); and the region between 2200 and 2500 nm.

Each discriminant model was then tested for accuracy by using it to predict the variety of samples in the validation set. A sample in the validation set was classified as a Riesling wine if its predicted value was between 0.5 and 1.5, and it was classified as Chardonnay if the value was between 1.5 and 2.5. The criteria for the cutoff selected were similar to those reported by others (*18*, *21*, *30*, *31*).

RESULTS AND DISCUSSION

Chemical Analysis. Table 1 shows the descriptive statistics for the chemical constituents analyzed in both commercial bottled wine varieties. The chemical composition of the wine samples was considered to be typical for Australian table wines (*32*). By comparison of the composition of the samples grouped by the two varieties, statistically significant differences in the mean values were found for the constituents alcohol, specific gravity, pH, and dry extract ($p < 0.05$).

Spectral Analysis. Figure 1 shows the visible and NIR spectra of the white wine samples analyzed. No obvious differences were detected from a visual observation of the spectra between the two white wine varieties in either the visible or NIR region. Both varieties have absorption bands at 1450 nm related to the O−H second overtone of water and ethanol, at 1690 nm related with either C−H$_3$ stretch first overtone or compounds containing C−H aromatic groups, at 1790 nm related with C−H stretch first overtone, and at 1950 nm with O−H stretch first overtone of water and ethanol (*8*, *33*). The absorption band at 2266 nm is likely related to C−H combinations and O−H stretch overtones and that at 2305 nm to C−H overtones (*33*). Absorptions at 2266 and 2302 nm are most likely C−H combination bands of methanol (*22*). Absorption bands at 1450, 1790, and 2266 nm were also reported to be associated with sucrose, fructose, and glucose in fruit juices (*34*). Absorption bands around 1900−2000 nm are also associated with S−H tones and those around 2150−2250 nm with C−S tones (*35*). Transforming the spectra by the second derivative inverts the spectra so that peaks become narrow valleys (*28*). The highest variations in the second derivative of the spectra can be seen in **Figure 2**, which shows the standard deviation for each wavelength, and were also around 1432, 1692, 2180, and 2278 nm. High standard deviations were also observed at 1552 and 1876 nm and are probably associated with the O−H and N−H overtones, respectively (*33*).
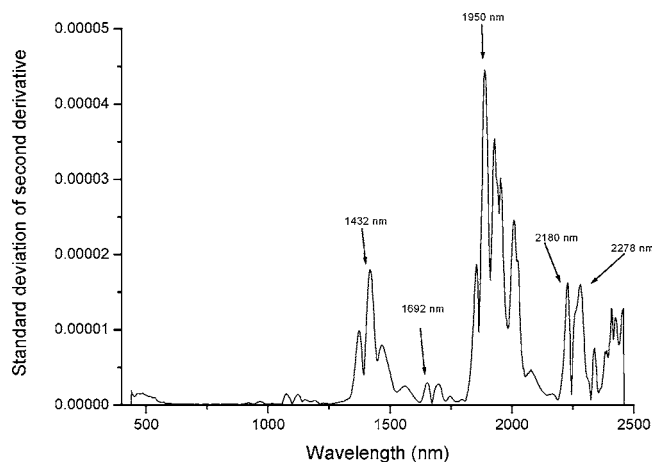
PCA. PCA was performed on the spectra (raw and second derivative, 400−2500 nm) to examine qualitative differences between the two commercial wine varieties. **Figure 3** shows the PCA scores (PC1 vs PC2) derived from the second derivative of the spectra of the samples. Generally, there was separation of the samples by variety; however, some samples did overlap. The samples used were commercially available bottles of wine and could not be completely verified in terms of their authenticity other than the claim made on the label. Australian wine industry regulations (*36*) state that a single varietal wine must contain a minimum of 85% of the variety as claimed on the label. It is therefore possible that some of the samples were not 100% of the variety as claimed, which might explain the overlap. Therefore, this result suggests that the discrimination between varieties is possible and that different spectral attributes of samples are associated with either characteristics of the variety or the typical wine-making style for each commercial label.

To investigate the basis for the observed spectral discrimination between the two wine varieties, the PCA eigenvectors were analyzed (see **Figure 4**). The first four PCs account for 95% of the variation in the spectra. PC1 explains 63% of the total variance in the samples, and the highest eigenvectors were found around 1430 nm associated with O−H absorption bands (second overtone), at 1892 nm with O−H stretch and C=O second-overtone combinations, at 1936 nm with O−H first overtone, and at 2234 and 2234 nm related to C−H and C=C tones, respectively (*33*). These spectral regions are characteristic of either water absorption (O−H overtones) (*33*), ethanol content (*8*, *33*), or sugars in the wine. PC2 explains 16% of the variation, and the highest eigenvectors were found around 1406 and 1950 nm, both related to O−H overtones due to water, and between 2000 and 2100 nm, related to both C−H and C=C tones (*33*). The eigenvector at 1406 nm is associated with sugar content, especially glucose and fructose (*34*). Therefore, it is suggested that particular chemical constituents, such as ethanol, water, sugars (glucose and fructose), phenolic compounds, lactic acid, and oxidation products, either in combination or alone, contribute the strongest influences that explain the basis for the observed discrimination between the two commercial varieties.

Discriminant Analysis. NIR spectra contain information about the chemical composition and physical state of the material under analysis, yielding structural information that constitutes the fingerprint of a sample (*12*, *13*). In general, supervised classification (e.g., discriminant analysis) is used to test similar known authentic samples. Central to this philosophy is the principle that, in relative terms, the spectra of samples of a given
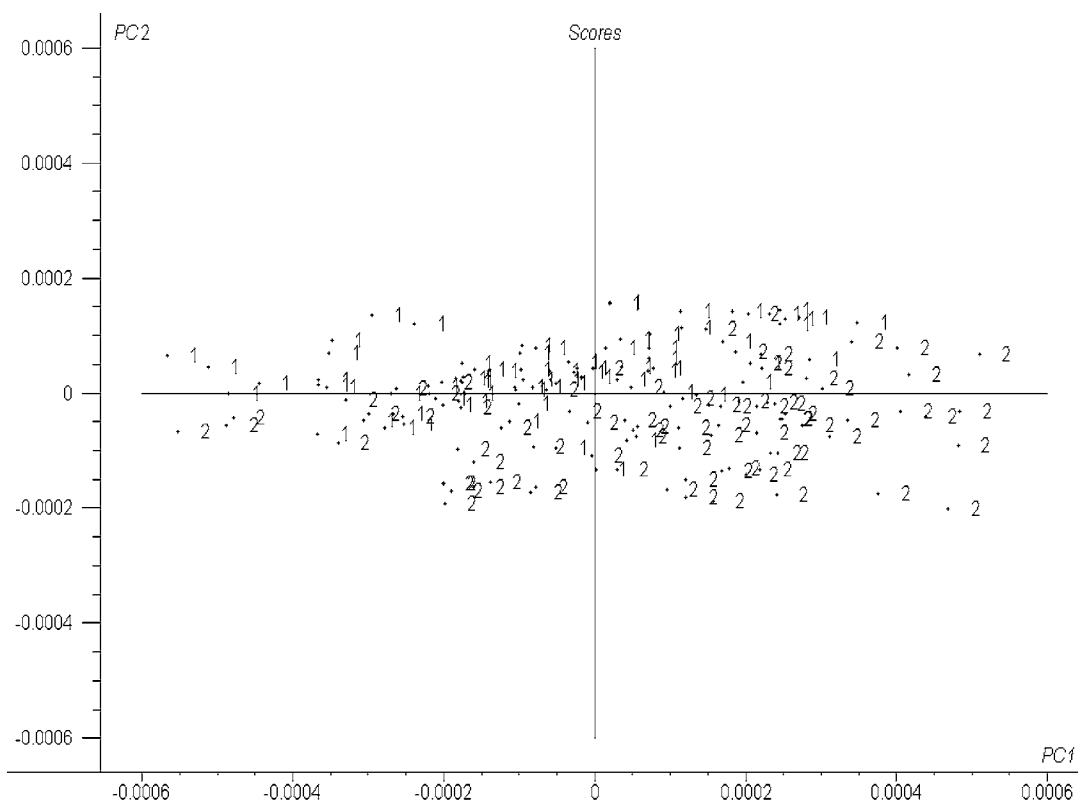
Figure 3. Sample score plot for PC1 and PC2 (second derivative, 400–2500 nm) for the white wines (1 = Riesling; 2 = Chardonnay).
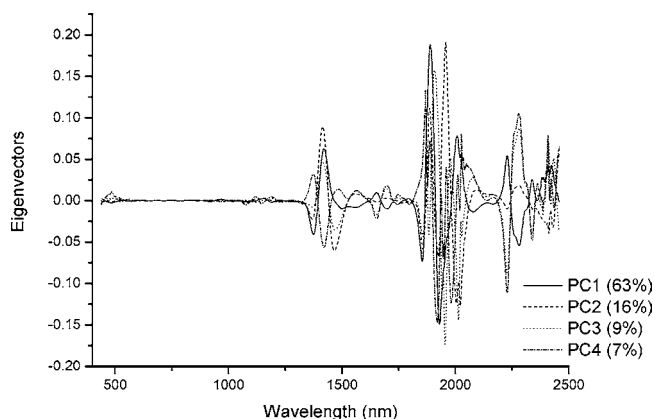

Figure 4. Eigenvectors for the PCA on the white wine samples analyzed (in parentheses is the amount of variation explained by each PC).

Table 2. Calibration Statistics for White Wine Varietal Origin Using DPLS Discriminant Models (Raw and Second Derivative) ($n = 136$)[a]

data type	wavelength range (nm)	R^2_{cal}	SECV	% of samples correctly classified in calibration	no. of loadings in optimal models
raw	400–750	0.94	0.19	98.5	10
	400–1100	0.96	0.18	99.2	11
	400–2500	0.90	0.28	97.1	12
	1100–2500	0.88	0.30	97.1	11
	2200–2500	0.85	0.26	97.8	9
second derivative	400–750	0.92	0.22	100	11
	400–1100	0.94	0.20	100	12
	400–2500	0.90	0.25	100	12
	1100–2500	0.88	0.27	99.2	12
	2200–2500	0.83	0.25	97.8	8

[a] R^2_{cal}, coefficient of determination of regression; SEC, standard error in calibration; SECV, standard error in cross-validation.

material are similar to each other but different from spectra of other materials (*12*).

Table 2 shows calibration statistics from DPLS regression models developed either on the raw spectra or after second derivative using various wavelength regions. The PCR regression models developed always showed the poorest calibration statistics compared with DPLS (data not presented). The results indicate that the DPLS models developed accounted for 83–96% (coefficient of determination $R^2_{cal} = 0.83$–0.96) of the variability for wine variety classification. In agreement with other authors, the optimal combination of spectral regions varied among regression methods (*20, 31*). Wavelength regions of 400–750, 400–1100, and 400–2500 nm gave the best calibration statistics depending on the data type used. In all of the cases, the inclusion of spectral information from the visible region was essential to obtain the optimum calibration for wine variety discrimination, despite the observation that the sample spectra did not visually appear to have any marked features in

this region (**Figure 1**). PLS loadings of the calibration models for the discrimination between varieties were similar to the eigenvectors described for the PCA analysis.

The results for the predictions of the wine variety using the best DPLS regression models selected from **Table 2** are summarized in **Table 3**. Riesling wines were classified correctly in 100% of cases; however, the classification for Chardonnay wines ranged from 96 to 100% depending on the wavelength range used. This may have been due to the probability that not all of the Chardonnay wines were 100% pure varietal. In fact, it was verified by the winemakers that some Chardonnay samples were not 100% pure and were blended either with Riesling (up to 5% in some cases) or with other white Australian varieties (e.g., Semillon and Sauvignon Blanc) according to Australian label integrity provisions. **Figure 5** shows the NIR predictions of commercial white varieties in the validation set using the best DPLS calibration (400–1100 nm and after second-derivative treatment of the spectra). For the Chardonnay

Vis-NIR Varietal Wine Discrimination

J. Agric. Food Chem., Vol. 51, No. 26, 2003 **7707**

Table 3. Optimum DPLS Discrimination Model for Prediction of White Wine Varietal Origin

data type	model spectra segment (nm)	variety	no. of samples correctly classified	no. of samples incorrectly classified	SEP[a]
raw	400–750	Riesling[b]	72	0	0.11
	400–1100	Riesling	72	0	0.13
	400–750	Chardonnay[c]	60	1	0.13
	400–1100	Chardonnay	61	0	0.11
second derivative	400–750	Riesling	72	0	0.11
	400–1100	Riesling	72	0	0.14
	400–750	Chardonnay	59	2	0.18
	400–1100	Chardonnay	61	1	0.14

[a] SEP, standard error of prediction. [b] $N = 72$ samples in the validation set. [c] $N = 61$ samples in the validation set.
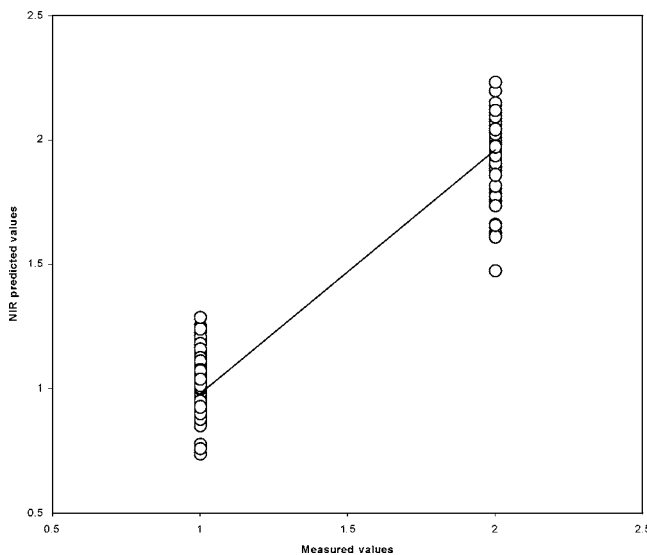
Figure 5. Prediction of commercial white wine varieties using DPLS regression (400–1100 nm) and second derivative (validation set).

samples, those classified as Riesling (i.e., predicted values below 1.5) had been blended with some Riesling, and those with predicted values above 2.5 had been blended with other varieties (samples with predicted values >2.5 were considered to be incorrectly classified by the models).

The ability of the NIR model to discriminate or identify varieties is based on the vibrational responses of chemical bonds to visible and near-infrared radiation. It is probable that the higher the variability between sample types in those chemical entities, which respond in these regions of the spectrum, the better the accuracy of the model. This suggests that it is not simply a specific constituent (e.g., ethanol, sugars, or phenolic compounds) but also the compositional characteristics of the wine as a whole that provides the necessary information for discrimination by NIR techniques.

Chemometric analyses together with spectroscopic methods are a very powerful tool for distinguishing groups of objects that have very similar properties such as white wines. The spectral and chemometric techniques studied here gave an excellent discrimination between samples of two varietal origins. The PLS loadings/PCA eigenvectors used for the discriminant model showed that the ethanol content of the sample is not the only parameter that explained the separation between the two varieties. Other chemical compounds or characteristics that could also contribute to the discrimination between varieties include sugars (glucose and fructose), phenolic compounds, or even nonvolatile compounds related with sensory attributes.

The results of this study suggest that NIR techniques might offer the possibility to analyze wine for authenticity of variety without the need for costly and laborious chemical and sensory analysis. However, in developing such models, it is known that the more properties (variables) used for classification, the more objects (samples) are needed to get a robust model. In the present study, only a limited number of samples and wine varieties were used and, therefore, caution must be considered in extending the applicability of the technique to discriminate between other varieties until further validation work is completed.

Conclusions. The results obtained in this study showed the potential of visible and near-infrared spectroscopy to discriminate by variety between commercially available bottles of Riesling and Chardonnay wine with accuracy up to 98%. These results also suggested that vis−NIR spectroscopy together with chemometric techniques, such as PCA or DPLS discriminant models, could be used by the wine industry for the identification of white wine varieties or their blends. The combination of the visible and NIR wavelength regions gave discriminant models with the best calibration statistics despite the observation that the spectra did not visibly show noticeable features in the visible region. The work reported here constitutes a feasibility study and requires further development with considerably more commercial samples of different varieties before its potential may be realized and adopted by the wine industry. Further studies are needed to improve the calibration specificity, accuracy, and robustness and to extend the discrimination to other wine varieties or blends.

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